A warm welcome to all of you to my course on Electronic Structure of Materials (PHY621). Electronic structure denotes the ground and excited states of the electrons, which determine the properties materials.

The objective of this course is to provide knowledge of basic principles that enable theoretical developments in electronic structure, familiarity with state-of-the-art computational methods with useful codes and experimental phenomena that can be explained using electronic structure theory.

We will emphasize on density functional theory (DFT), which makes it possible to use independent electron approximation to determine exact ground state properties of many-body electron systems. Due to its versatility to study diverse structures and chemistries, DFT has become the predominant method to study properties of quantum materials. In this course, we will focus on the capabilities as well as mention the short comings of DFT.

This is the first handout for this course. Some details regarding the course content, functioning of the course and the evaluation criteria are summarized here. You are requested to read this document as they will be followed during the course unless otherwise mentioned in the class.

Instructor:
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Classes: on WF 10:30-12:00

Office hour: by appointment through email (in my office).

Books:

- Richard M. Martin, **Electronic Structure: Basic Theory and Practical Methods** (Cambridge University Press)
- Feliciano Giustino, **Materials Modelling using Density Functional Theory** (Oxford University Press)
- Neil Aschroft and N. David Mermin **Solid State Physics** (Cengage Learning India

Broad course description:

- Quantum theory and origin of electronic structure, Emergence of quantitative calculations, Electronic structure theory and properties of quantum materials
- Crystal structures, reciprocal lattice and Brillouin zone, Electrons in periodic solids, Bloch's theorem, nearly-free electron model, energy bands, Fermi surfaces
- The independent electron approximations, Born-Oppenheimer approximation, Hartree and Hartree-Fock approximation, correlation hole and energy

- Foundation of density functional theory, Thomas-Fermi model; the Hohenberg-Kohn theorems, the Kohn-Sham auxiliary system; exchange and correlation energy functional, LDA, GGA, meta-GGA, hybrid functional
- Pseudopotential method, orthogonalized Plane Wave (OPW) method, Norm-conserving pseudopotential, Ultrasoft pseudopotential, augmented plane wave (APW) method
- Tight-binding method, Korringa-Kohn-Rostoker (KKR) method, linear muffin tin orbital (LMTO) method, full-potential method, coherent potential approximation (CPA)
- Quantum molecular dynamics, Born-Oppenheimer molecular dynamics, Car-Parinello molecular dynamics
- Application of density functional theory; calculations of materials properties and response functions; electronic structure, band gap, phonon dispersion, dielectric, thermal properties; Wannier functions, polarization, Berry phase, topological properties; application of electronic structure methods to materials design

Prerequisite:

- Condensed Matter Physics-I (PHY543) for masters and undergraduate students
- None for the PhD students
- Familiarity with programming language (such as Python, Fortran), scripting language (such as bash) would be helpful but not necessary

Grading:

- There will be a term paper and the endsem exam. Each of these will carry 50% of the total weight for this course.
- The topic for the term paper can be chosen by mutual interest. The paper should describe a general problem in depth within the electronic structure theory with appropriate literature references. It could be an application to an experimental measurement or analysis, or a computational project carried out during the course. It does NOT have to be original research, but it must be original work on the part of the student. The paper should be prepared in Phys. Rev. B format (preferably in LaTeX) and submitted before the endsem exam.
- Attending the classes and the exam is compulsory for passing this course.